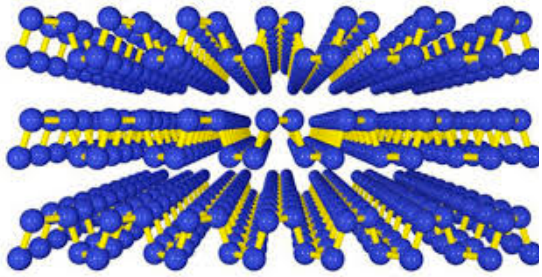
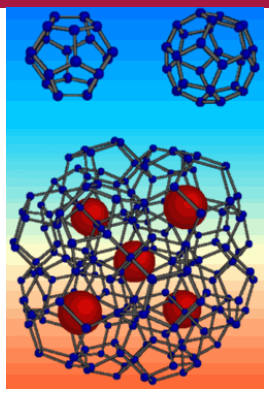
Science and Mathematics
2016 Colloquium Series

College of Integrative Sciences and Arts
ARIZONA STATE UNIVERSITY

"Computational materials research & applications in nano-electronics and renewable energies"



Phosphorene



Si clathrates

All are welcome!
Wednesday
August 31, 2016

3:00-4:00
Refreshments 2:45

SANCA 130

Xihong Peng

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College of Integrative Sciences and Arts
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First-principles electronic structure calculations are applicable to solving problems across various fields, ranging from physics and chemistry to material sciences and engineering. They play an essential role in modern scientific research and explorations. In this talk, I will outline my recent research in two particular nano-materials: phosphorene and Si clathrates. (a) Phosphorene, a recently fabricated two dimensional puckered honeycomb structure of phosphorus, showed promising properties for applications of nano-electronics. Our group have recently explored how size, edge/surface passivation and mechanical strain affect the properties of the monolayer phosphorene and obtained a picture on the interplay of size, passivation and strain on the electronic properties of this nanomaterial. (b) With increasing concerns regarding energy resource depletion, interest has arisen in the development of environmentally clean and safe processes that are capable of expanding our energy infrastructure. Our group conducted materials research through vigorous collaborations with experimentalists in areas such as Li-ion batteries, fuel and solar cells. Here I will provide an overview on the project of Si clathrate.

The Colloquium Series is funded by the Faculty of Science and Mathematics, CISA